Methodology 1

Machine Learning 2019
mlvu.github.io

offline machine learning: the basic recipe

next lecture:
Prepare your data

Problem to a **standard task.**
Classification, Regression, Clustering, Density estimation, Generative Modeling, Online learning, Reinforcement Learning, Structured Output Learning

Choose your **instances** and their **features**.
For supervised learning, choose a target.

Choose your **model class**.
Linear models, Decision Trees, kNN,

Search for a good model.
Usually, a model comes with its own search method. Sometimes multiple options are available.

today:
Evaluate your model

Here is the basic recipe for machine learning again. This week, we'll discuss what happens before and after. Today: once you've trained some models, how do you figure out which of them is best?

methodology

part 1:

Performing an experiment
Model selection, hyperparameter selection

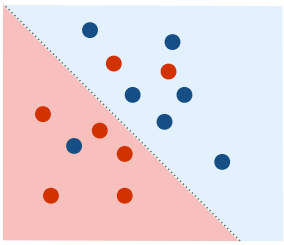
What to report (classification)
Accuracy, Confusion matrices, AUC, Coverage matrices

part 2:

What to report (regression)
Bias and variance, statistics

The no-free-lunch theorem and principle
Which model is the best in general?

binary classification



Positive class

Negative class

The classifier is a detector for the positive class.

error: 3/14

accuracy: 11/14

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We'll focus mostly on binary classification today (two-class classification). In this case, we can think of the classifier as a detector for one of the classes (like spam, or a disease). We tend to call this class positive. As in "testing positive for a disease."

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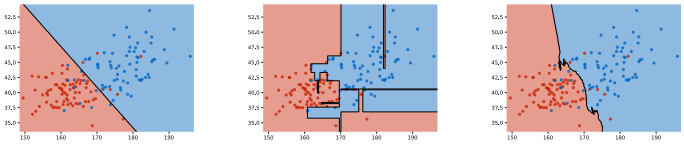
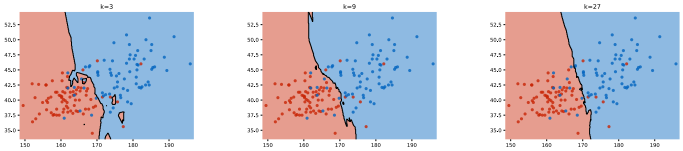
comparing models

linear vs. decision tree vs. kNN



different values of the *hyperparameter* k



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You compare models to figure out which is the best. Ultimately, to choose which model to you want to use in *production*. (This could be literally the production version of a piece of software, or just the model whose predictions you decide to trust ion the future.)

Sometimes you are comparing different models types, but you might also be comparing different ways of configuring the same model type. For instance in the kNN classifier, how many neighbours (k) should we look at to determine our classification?

With the 2D dataset, we can look at the decision boundary, and make a visual judgment. Usually, that's not the case: our feature space will have hundreds of dimensions, and we'll need to *measure* the performance of a model.

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performing an experiment

Train classifier **A**, Train classifier **B**

Compute the *error* of **A**, compute the *error* of **B**

error = proportion of mistakes

The lower the error, the better the model

On which data do we compute the error?

How do we eliminate random effects?

Is error the best metric to use?

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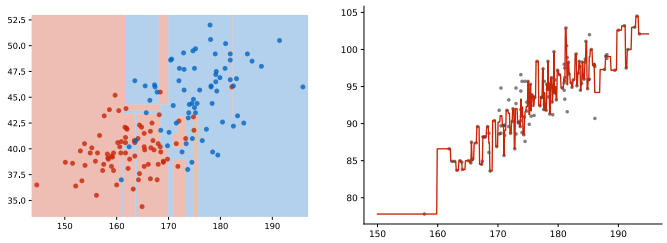
Here is the simplest, most straightforward way to compare two classifiers. You just train them both, so see how many examples they get wrong, and pick the one that made fewest mistakes. This is a very simple approach, but it's basically what we do.

We just need to consider **a few questions**, to make sure that we can trust our results.

Overfitting



We've already seen what happens when you evaluate on the training data. A model that fits the training data perfectly may not be much use.

Never judge your performance on the training data

the test set

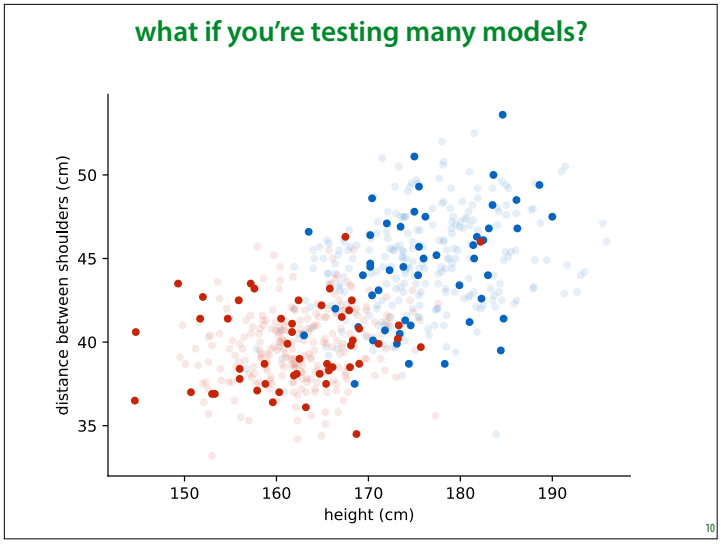
training data	test data

The proportion is not important, the absolute size of the test data is.

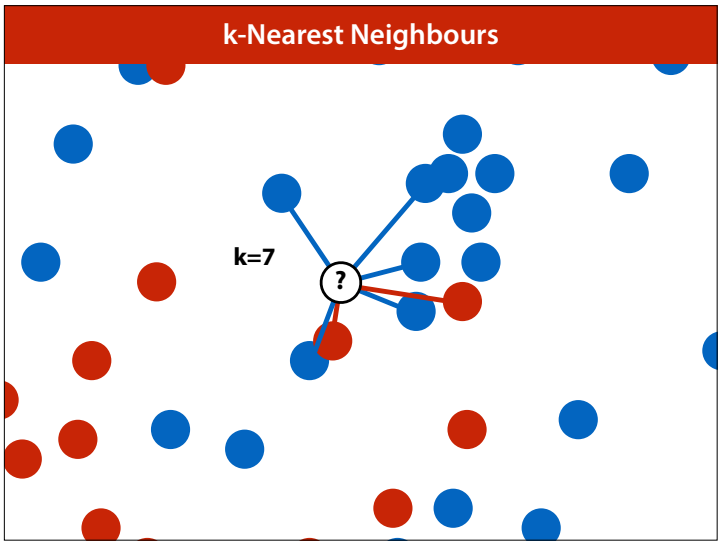
We should aim to have at least 500 examples in the test data (about 10000 is ideal).

So the first thing we do in machine learning is withhold some data. We train our classifiers on the training data and test on the test data. That way, if we get good performance, we know that we're likely to get a good performance on future data as well, and we haven't just memorised random fluctuations in the training data.

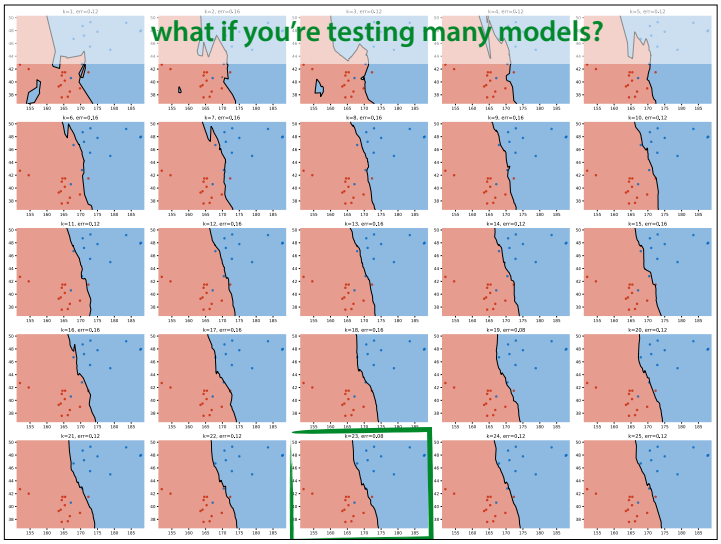
How should we split our data? The most important factor is the size in instances of the test data. The bigger this number, the more precise our estimate of our model's error. Ideally, we separate 10000 test instances, and use whatever we have left over as training data. Unfortunately, this is not always realistic. We'll look at this a little more in the second half.



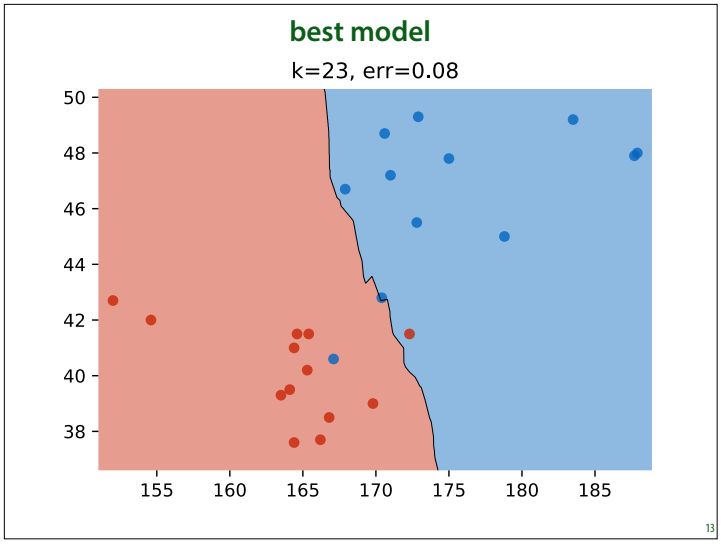
But even if we withhold some test data, we can still go wrong. Let's look at the data from the first lecture, take a small subset (to emphasize the effect) and see what happens when we test many different models.



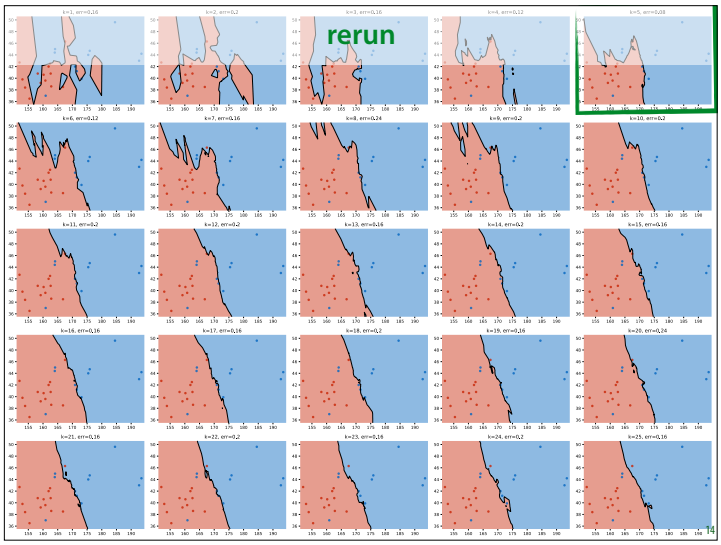
Remember, the kNN classifier just takes the k nearest points from the training data and assigns the class most prevalent among those points.



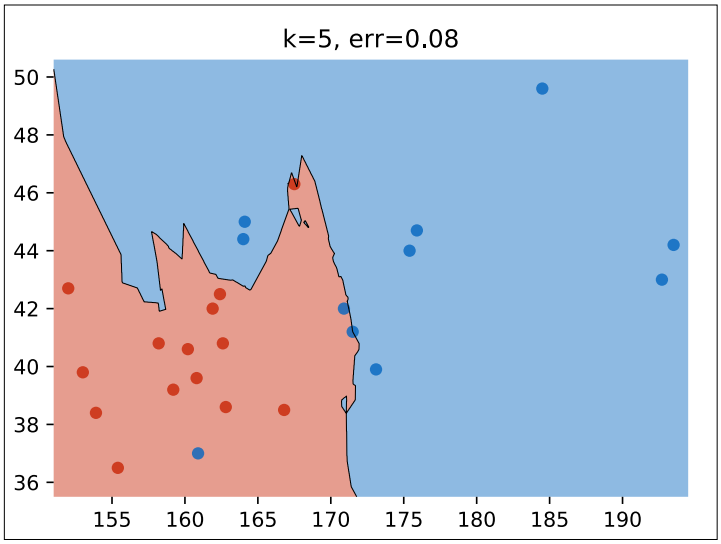
Here we've tested 25 different values of k on the same test data (using quite a small test set to illustrate the idea).

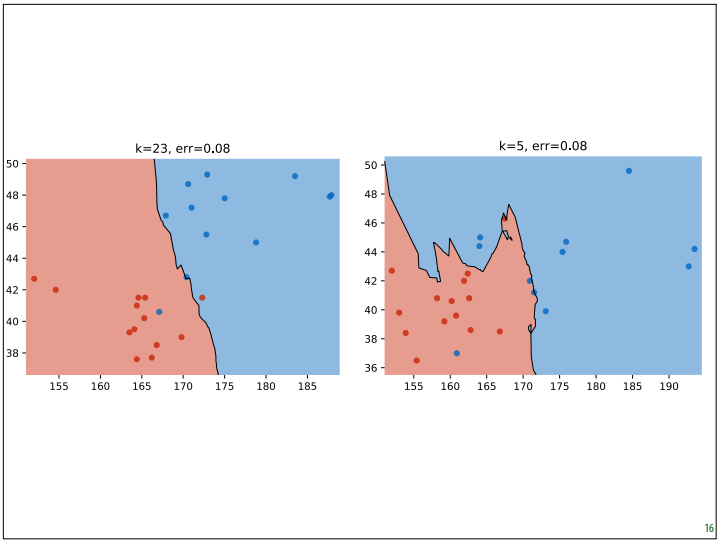


Here is the best run. Should we conclude that k=23 is definitely a better setting than k=22 or k=24?



In this case, we have some more data from the same source, so we can do the whole experiment again in fresh data. Usually, this isn't the case, of course, and we use all the data we have.





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The same source of data, the exact same procedure, and these are the results. Clearly, we can't trust that these models are actually learning the shape of the data.

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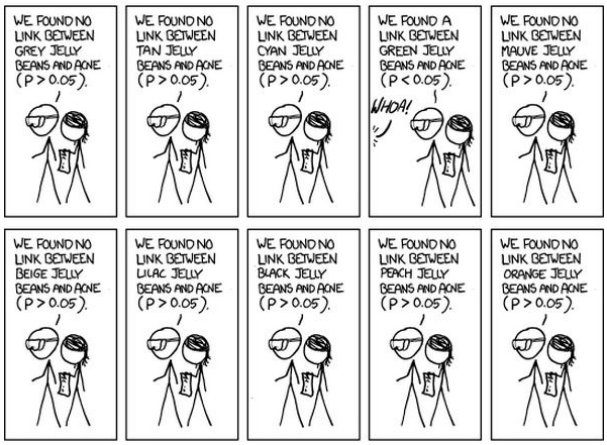
conclusion: we're overfitting again



source: xkcd.com/882

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This is essentially the overfitting problem again. Our method of choosing the hyperparameter **k** (or the model itself) is just another learning algorithm. By testing so many values of k on the test data, we are overfitting our choice of k on the test data.

This is an instance of the multiple testing problem in statistics. We're testing so many things, that the likelihood of a noticeable effect popping up by chance increases. We are in danger of ascribing meaning to random fluctuations. The simple answer to the problem of multiple testing is **not to test multiple times**.

see also: **https://www.explainxkcd.com/wiki/index.php/882:_Significant**

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evaluation: the modern recipe

Split your data into train and test data.
Sample randomly. At least 500 examples in your testset.

Choose your model, hyper parameters, etc. only using the training set.
Save your test set until the very last minute. Don't use it for anything.

State your hypothesis
i.e. *kNN with k=7 beats existing model X*, or *kNN with k=7 is better than kNN with k = 12*

Test your hypothesis **once** on the test data
This is usually at the very end of your project when you write your report or paper.

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There are many different approaches to machine learning experimentation, and not every paper you see will follow this approach, but we believe this is the simplest way to get reliable results.

It's important to mention in your paper that you followed this approach, since the reader can't usually see it from the presented results.

Don't re-use your test data

Just to emphasize the important point: the more you use the test data, the less reliable your conclusions become. Figure out what the end of your project is, and do not touch the test data until the end.

In really important and long-term projects, it's not a bad idea to withhold multiple test sets. This allows you to still test your conclusions in case you've ended up using the original test data too often.

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reusing your test data

Causes you to pick the wrong model

Inflates your performance estimate

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Not only does reusing test data mean that you pick the wrong model, it also means that the error estimate you get is probably much lower that the error you would actually get if you gathered some more test data.

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validation set

During model and hyperparam. selection:

- train on: training
- test on: validation

Final run:

- train on: training validation
- test on: test

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This means that you need to test which model to use, which hyperparameters to give it, and how to extract your features **only on the training data**. In order not to evaluate on the training data for these evaluations, you usually split the training data **again**: into a training set and **a validation set**.

Ideally, your validation data is the same size as your test set, but you can make it a little smaller to get some more training data.

This means that you need to **carefully plan your research process**. If you start out with just a single split and keep testing on the same test data, there's no going back (you can't unsee your test data). And usually, you don't have the means to gather some new dataset.

not this

	dataset 1	dataset 2	dataset 3
other method 1	0.15	0.08	0.27
other method 2	0.11	0.10	0.29
ours (k=1)	0.89	0.45	**0.23**
ours (k=2)	0.09	0.23	0.70
ours (k=3)	**0.08**	0.45	0.57
ours (k=4)	0.15	0.56	0.32
ours (k=5)	0.57	0.09	0.88
ours (k=6)	0.58	**0.07**	0.89

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Here what you might come across in a (bad) machine learning paper. In this (fictional) example, the authors have re-used the test set to select their hyperparameters. They are claiming that their model beats every baseline, because their numbers are higher (for specific hyperparameters).

These numbers create three impressions that are not actually validated by this experiment:

- That the authors have a better model that the two other methods shown.
- That if you want to run the model on dataset 1, you should use k=3
- That if you have data like dataset 1, you can expect an error of 0.08.

None of these conclusions can be drawn from this experiment, because we have not ruled out multiple testing.

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but this

	dataset 1	dataset 2	dataset 3
other method 1	0.15	0.08	0.27
other method 2	**0.11**	0.10	0.29
k	3	5	2
ours	**0.11**	0.11	**0.24**

"The hyperparameter k was chosen based on a validation set split off from the training data. The test data was used only once."

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Here is what we should do instead. We should use the training data to select our hyperparameters, make a single choice, and then estimate the accuracy of only that model.

NB: The numbers have changed, because in the previous example we gave ourselves an advantage by multiple testing. These number are lower, but more accurate. (I made these numbers up, but this is the sort of thing you might see)

Now, we can actually draw the conclusions that the table implies:

- On dataset 3, the new method is the best.
- If we want to use the method on dataset 3 (or similar data) we should use k=2
- If our data is similar to that of dataset 3, we could expect a performance around 0.24

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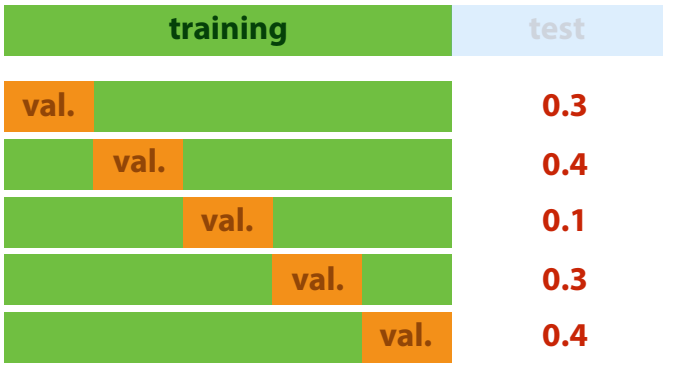
cross-validation



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After you've split off a test and validation set, you may be left with very little training data. If this is the case, you can make better use of your training data by performing **cross-validation**. You split your data into 5 chunks ("folds") and for each specific choice of hyperparameters that you want to test, you do five runs: each with one of the folds as validation data. You then average the scores of these runs.

This can be costly (because you need to train five times as many classifiers), but you ensure that every instance has been used as a training example once.

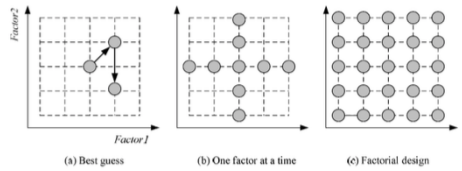
After selecting your hyperparameters with crossvalidation, you still test once on the test data.

You may occasionally see papers that estimate error of their finally chosen model by cross validation as well, but this is a complicated business, and has fallen out of fashion.

which hyperparameters to try?

Up to you:

- trial-and-error (intuition)
- grid search
- random search (remember?)



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Which values should we try for the hyperparameters? So long as we make sure not to look at our test set, we can do what we like. We can try a few values, we can search a grid of values exhaustively, or we can even use methods like random search, or simulated annealing.

Is an error of 0.05 good?

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Now that we know how to properly estimate the classification error of our model, let's see what it means.

Imagine that somebody tells you about a machine learning project they're doing, and they proudly state that they get a classification error (on their validation set) of 0.01 (5% of the validation set is misclassified). Should you be impressed?

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example: breast cancer screening

For an example, let's look at a recurring discussion in the Dutch media: should all women over 50 be screened for breast cancer. This is an analogy for classification: the instances are people and the target label is "has cancer" or "has no cancer."

The answer depends on the classifier. Let's say that we get 95% accuracy. Is that good? It depends on two questions.

source: **https://www.volkskrant.nl/wetenschap/redt-preventieve-screening-op-borstkanker-levens~a3761451/**

it depends

Class imbalance How much more likely is a Positive example than a Negative example?

Cost imbalance How much worse is a mislabeled Positive example than a mislabeled Negative example?

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Imagine a classifier for breast cancer with 95% accuracy. This may seem impressive at first sight, but the prevalence of great cancer among women over 50 (the population that is regularly tested) is about 1%. This means that **a classifier that classifies nobody as having cancer** gets 99% accuracy. The range of accuracies that are interesting at all is between 99% and 100%.

Another reason to mistrust accuracy (besides class imbalance) is **cost imbalance**. There are two types of misclassification: diagnosing a healthy person with cancer and diagnosing a person with cancer as healthy. Both come with a cost but not the same cost. Spam classification is another example: both misclassifications should be avoided, but having a genuine email land in your spam is much worse than having to delete a spam email from your inbox.

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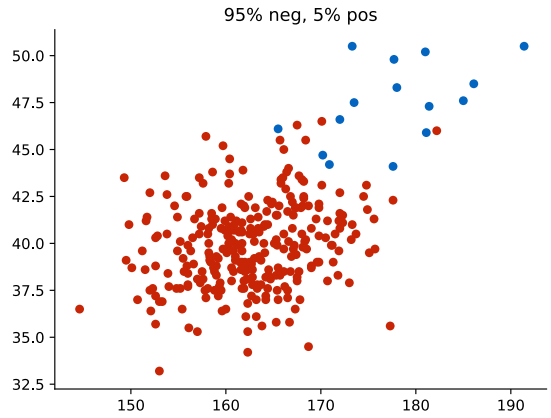
class imbalance



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Here is a pretty imbalanced dataset (though still not as imbalanced as the cancer/not cancer problem). It looks pretty difficult. What would be a good performance on this task?

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class imbalance

other method 1	0.15
other method 2	0.1
majority class	**0.05**
ours	**0.05**

Majority class classifier Assigns all instances the class that is most prevalent in your data.

Example of a **baseline**.

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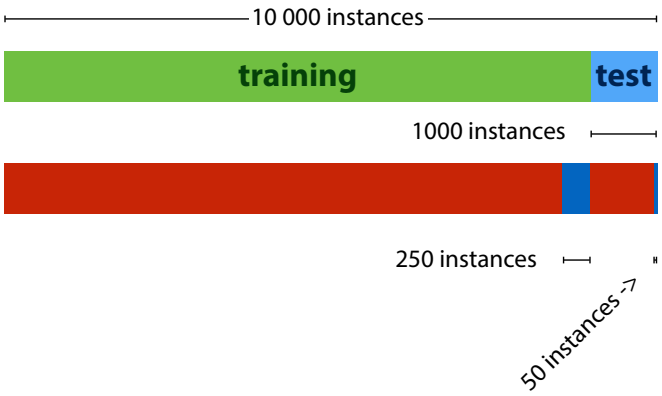
Something like an error of 0.05 might sound pretty good, but on an imbalanced dataset like this, there is a very simple classifier that gets that performance easily: the **majority class classifier**

The majority class classifier is an example of a **baseline**, a simple method that is not meant to be used as a real model, but that can help you calibrate the performance scores. In this case, it tells you that you're really only interested in in the range from 0 to 0.05. Any higher error than that is pretty useless.

class imbalance



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Here is another way that class imbalance can screw things up for you. You might think you have a pretty decent amount of data with 1000 instances. However if you split off a test set of 1000 instances, you're left with just 50 instances of the positive class in your data. Practically, your final evaluation will just be a question of how many of these 50 positives you detect. This means that you can really only have 50 "levels of accuracy" that you can distinguish between.

You can make a bigger test set of course (and you probably should) but that leads to problems in your training data. Since you're essentially building a detector for positives, it doesn't help if you can only give it 100 examples of what a positive looks like.

In the next lecture, we'll look at some tricks we can use to boost performance on such imbalanced data.

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cost imbalance

disease diagnosis Sending a sick person home vs applying invasive tests to a healthy person

spam classification Deleting a valid email vs showing the user a single spam email

detecting financial fraud Having an expert review a non-fraudulent transaction vs missing a fraud in progress

Domain-specific evaluation function: dollars lost, time lost, lives lost, etc.

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The second thing we need to consider when interpreting errors is cost imbalance.

In all these cases, one misclassification one way costs much more than a misclassification the other way. But both cost *something*. The time of an expert reviewer is not free, even though five minutes of his time may be much cheaper than the cost of letting a single fraud go unchecked.

If you're lucky, both types of misclassification have the same unit, and you can turn your error (an estimate of the number of misclassifictions) into a domain specific evaluation function (like estimated dollars lost, or time saved). **You simply assign a cost to each type if misclassification, and multiply it by how often that misclassification occurs in the test set.**

If the units are not the same (money saved vs lives saved) making such a choice can seem very unethical. On the other hand, any classifier you decide to deploy *implicitly* makes such a choice. Even if you decide not to use machine learning, the alternative (a doctor using their own judgement) is also a "classifier", with its own cost balance.

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other performance metrics

Confusion matrix

True positive rate, false positive rate

ROC plot

Precision, recall

Area under the curve

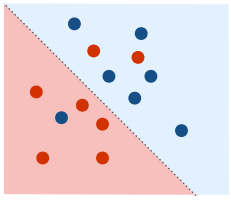
Coverage matrix

33

The best thing to do under class and cost imbalance, is to look at your performance in more detail. We'll look at six different ways to measure classifier performance.

Most of these are only relevant if you have class or cost imbalance. If you have a nice, balanced dataset, it's likely that error or accuracy is all you need.

confusion matrix



actual \ predicted	pos	neg	
pos	6	1	7
neg	2	5	7
	8	6	

34

This is s a **confusion matrix** (also known as a contingency table). It doesn't give you a single number, so it's more difficult to compare two classifiers by their confusion matrices, but it's a good way to get insight into what your classifier is actually doing.

The margins of the table give us four totals: the actual number of each class present in the data, and the number of each class predicted by the classifier.

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with class imbalance

actual \ predicted	pos	neg	
pos	385	0	385
neg	15	0	15
	400	0	

35

Here we see the confusion matrix for the majority vote baseline in a problem with high class imbalance.

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metrics

actual \ predicted	pos	neg
pos	TP	FN
neg	FP	TN

accuracy
(TP + TN)/ total

true positive rate
TP/(TP + FN)

false positive rate
FP/(FP + TN)

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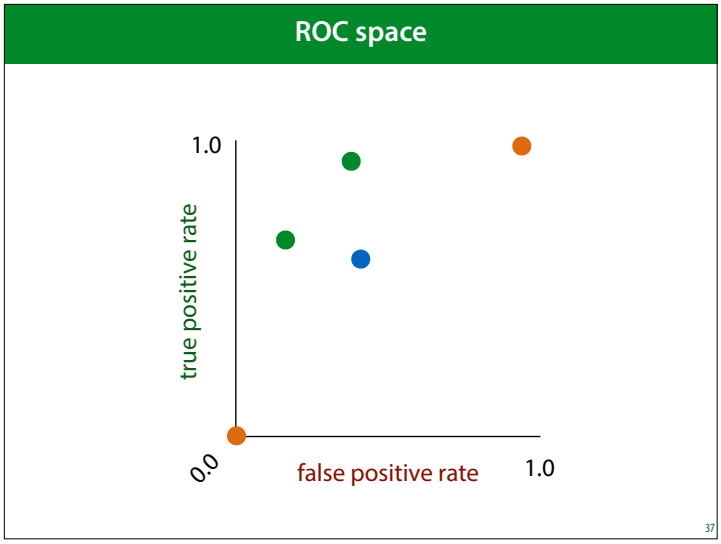
We call accurately classified instances **true positives** and **true negatives**. Misclassifications are called **false positives** and **false negatives**.

Many performance measures can be computed from the confusion matrix (including the error and accuracy).

A good pair of metrics to consider, especially when we have class imbalance, is the true and false positive rate:

true positive rate: what proportion of the actual positives did we get *right*. The higher the better. I.e. How many of the people with cancer did we detect.

false positive rate: what proportion of the actual negatives did we get *wrong* (by labelling them as positives). The lower the better. I.e. How many healthy people did we diagnose with cancer.

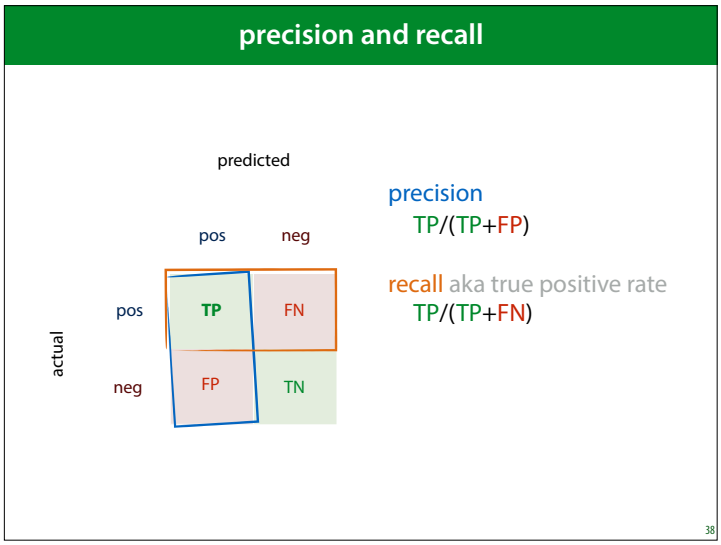


The TPR and the FPR are competing objectives, which we often have to trade off. Since we don't know how to balance them (this depends on domain specific preferences), we can visualize both objects together in the plane. Each classifier represents a point.

The points in the corners represent the classifier that designates everything as positive and the classifier that designates nothing as positive.

Whether we prefer the left or the right green classifier depends on our preferences. What ever our preference, we always prefer either green classifier to the blue classifier.

ROC stands for **receiver-operating characteristic**, a leftover from its invention in WWII, to improve the detection of Japanese aircraft from radar signals.

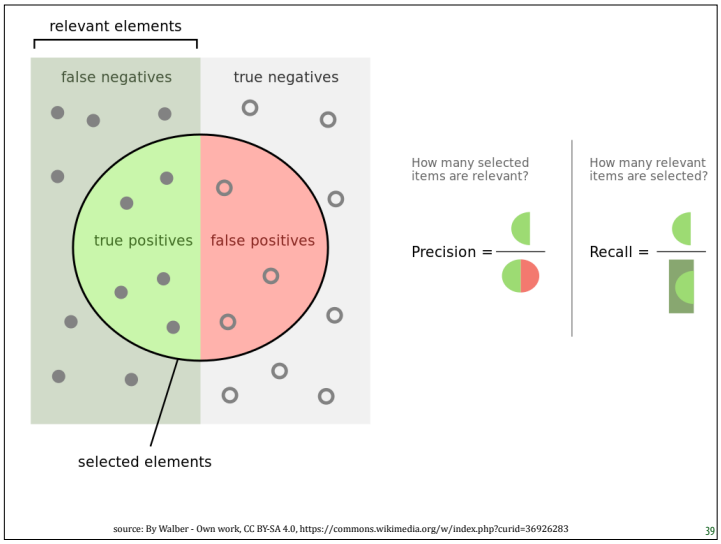


Precision and recall are two other metrics that express a similar tradeoff.

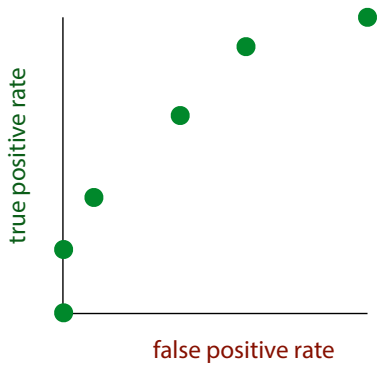
Precision: what proportion of the returned positives are actually positive?

Recall: what proportion of the existing positives did we find?

These can also be plotted in 2 axes. For now, we'll stick with the ROC space.



setting a threshold



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Imagine if we had one classifier, but we could control how eager it was to call things positive. If we made it entirely timid, it would classify nothing as positive and start in the bottom left corner. As it grew more brave, it would start classifying some things as positive, but only if it was really sure, and its true positive rate would go up. If we made it even more daring, it would start getting some things wrong and both the tpr and the fpr would increase. Finally, it would end up classifying everything as positive, and end up on the top right corner.

The curve this classifier would trace out, would give us an indication of its performance, *independent* of how brave or how timid we make it. How can we build such a classifier?

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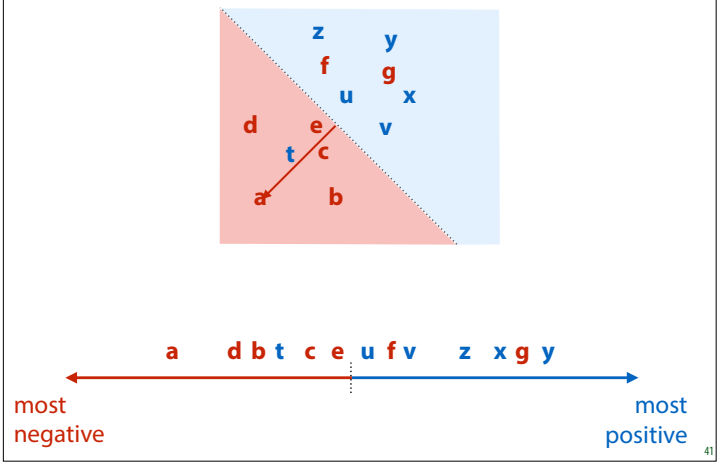
ranking classifiers



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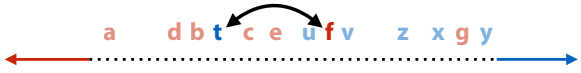
We can achieve this by turning a regular classifier into a **ranking classifier** (also known as a **scoring classifier**). A ranking classifier doesn't just provide classes, it also give a score of *how* negative or *how* positive a point is. We can use this to rank the points from most negative to most positive.

How to do this depends on the classifier. Here's how to do it for a linear classifier. We simply measure the distance to the decision boundary.We can now scale our classifier from timid to bold by moving the decision boundary from left to right.

After we have a ranking, we can scale the eagerness of the classifier to make things positive. by moving the threshold (the dotted line) from left to right, the classifier becomes more eager to call things negative. This allows us to trade off the true positive rate and the false positive rate.

---

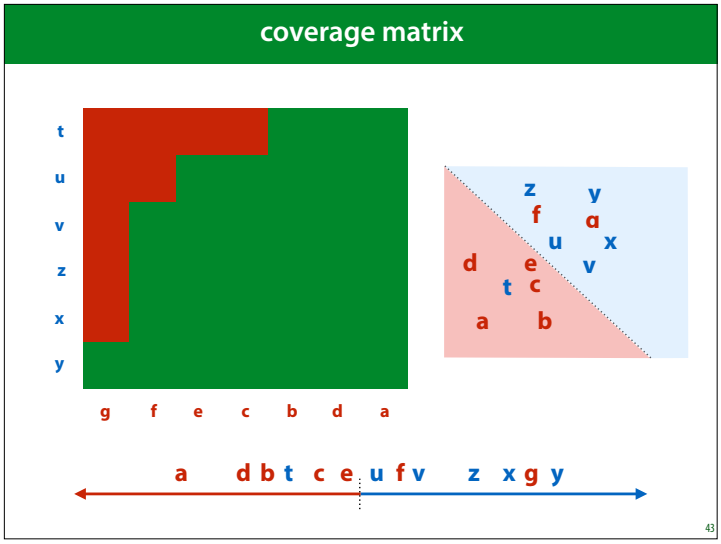
ranking error



42

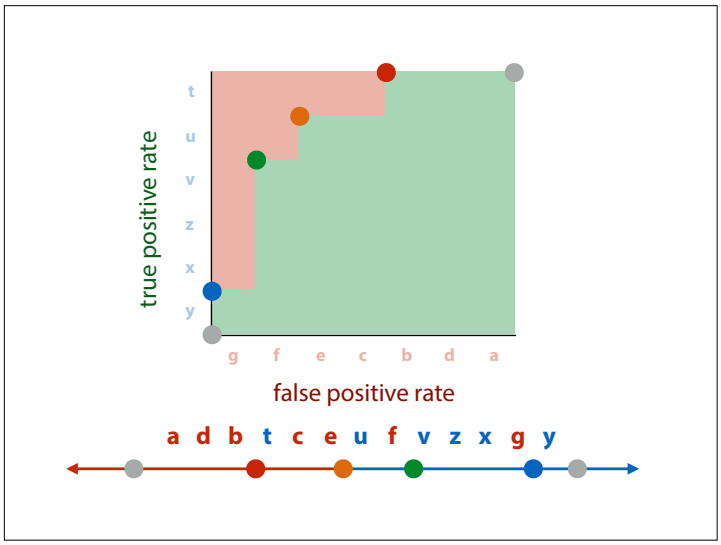
Now, we can't test a ranking on our test data, because we don't know what the correct ranking is. We don't get a correct ranking, just a correct *labeling*. However, we can indicate for specific pairs that they are ranked the wrong way around: all pairs of different labels. For instance, **t** and **f** form a ranking error: **t** is ranked as more negative than **f**, even though **t** is positive and **f** is negative.

Note: a ranking error is a *pair* of instances that is classified the wrong way around. A single instance can be part of multiple ranking errors.

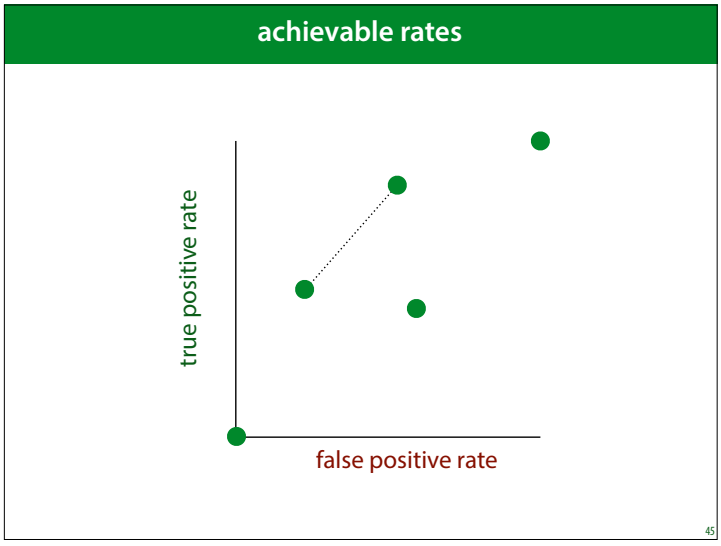


We can make a big matrix of all the pairs for which we know how they should be ranked: negative points on the horizontal axis, positive on the vertical. The more sure we are that a point is positive, the closer we put it to the bottom left corner. This is called a **coverage matrix**. We color a cell green if the corresponding points are ranked the right way round, and red if they are ranked the wrong way round.

Note that the proportion of this table that is red, is the probability of making a ranking error.

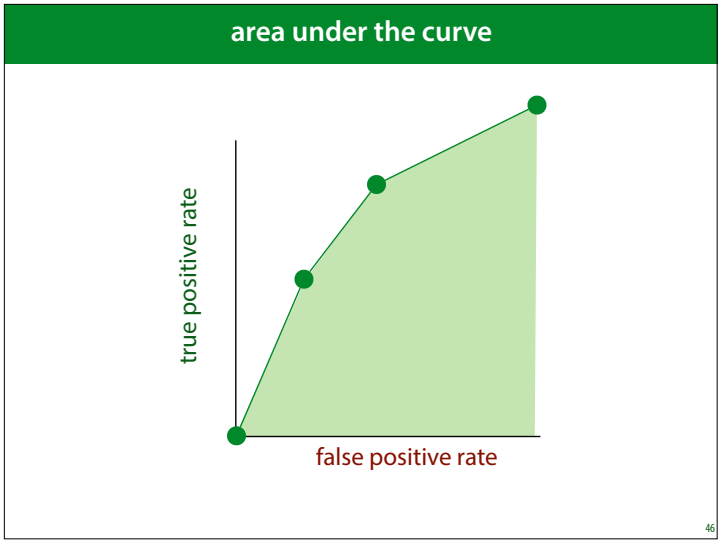


The coverage matrix shows us exactly what happens to the true positive rate and the false positive rate if we move the threshold from the right to the left. We get exactly the kind of behaviour we talked about earlier. We move from the all-positive classifier step by step to the all-negative classifier.



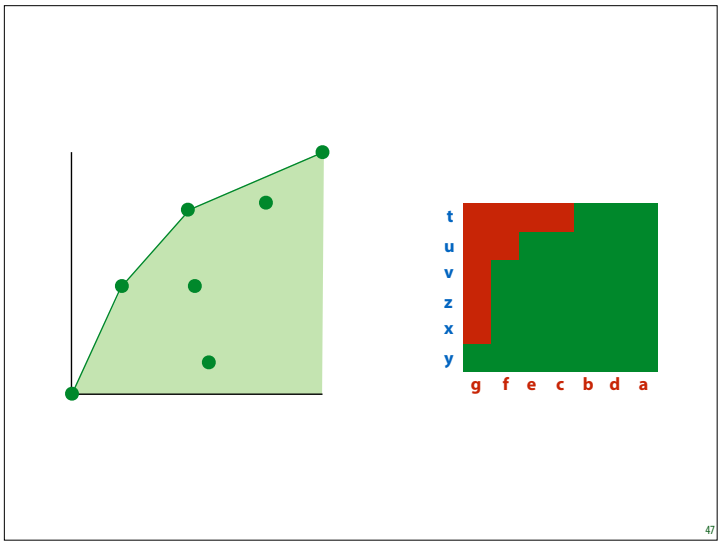
If we draw a line between two classifiers we know we can create, we can create a classifier for every point on that line simply by picking the output of one of the classifiers at random. If we pick with 50/50 probability we end up precisely halfway between the two.

If we vary the probability we can get closer to either classifier.

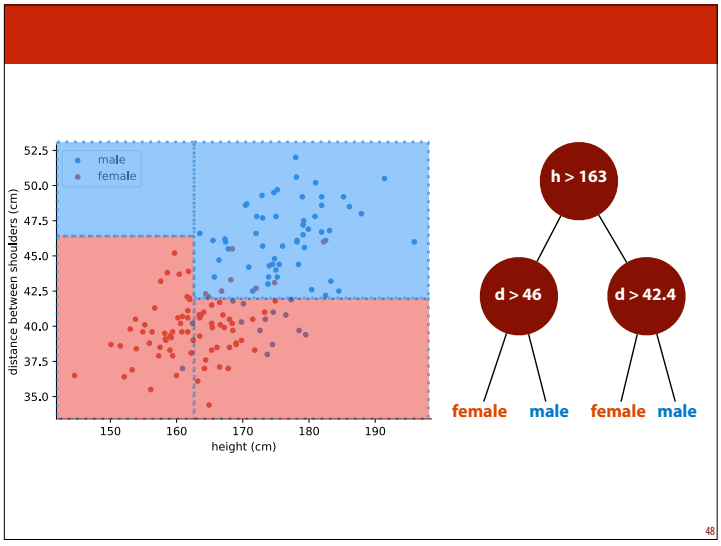


The area under the curve (AUC) of classifiers that we can create is a good indication of the quality of the classifier. The bigger this area, the more useful classifiers we can achieve.

The AUC is a good way to compare classifiers with class or cost imbalance, where we don't know what our preferences are.



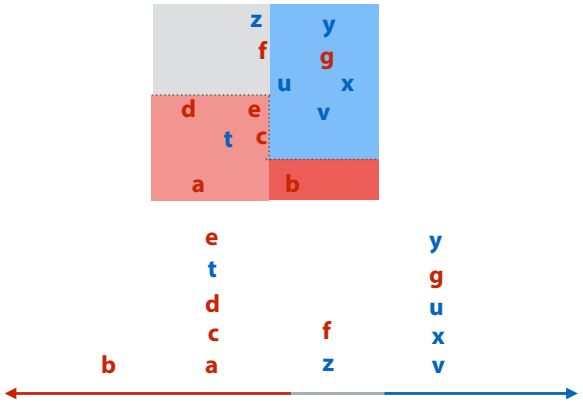
As we saw before: normalizing the coverage matrix gives us the ROC space (barring some small differences that disappear for large datasets). The area under the ROC curve is an estimate of the green proportion of the coverage matrix. This gives us a good way to interpret the AUC. **The AUC is an estimate of the probability that a ranking classifier puts a given pair of positive and negative examples in the correct order.**



To re-iterate, **how we get a ranking from a classifier depends entirely on the model**. Let's look at one more example: the tree classifier that we saw earlier. Again, we'll discuss the actual algorithm for training decision trees later. For now, we'll just

Remember that the decision tree classifier splits the feature space into rectangular **segments** and assigns each a class.

ranking decision tree



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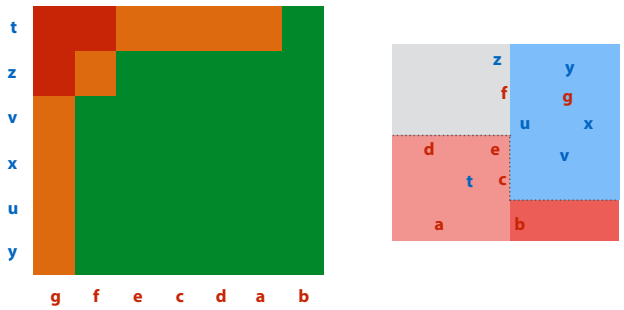
In this example we have an instance space that has been split into four segments by a decision tree. We rank the segments by the proportion of positive points. We then put all points in one region on the same level in the ranking.

In this example, **b** is more negative than **a**, because **b**'s segment contains only negative examples, whereas **a**'s segment contains a mix of positive and negative examples.



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This means that for some pairs (like **f**,**z**), the classifier ranks them as "the same". We'll color these **orange**.

For large datasets, these regions will not contribute much to the total area under the curve.

---

important points

The confusion matrix and all metrics derived from it are metric for a *single* classifier.

AUC is a metric for a *collection of classifiers*, usually derived from a ranking classifier.

How to turn a classifier into a ranking classifier, depends on the type of classifier.

For linear classifiers, take the distance to the decision boundary
For tree classifiers, sort by class proportion in each segment

AUC is a good metric if we don't know the relative importance of the classes, or if the classes are unbalanced.

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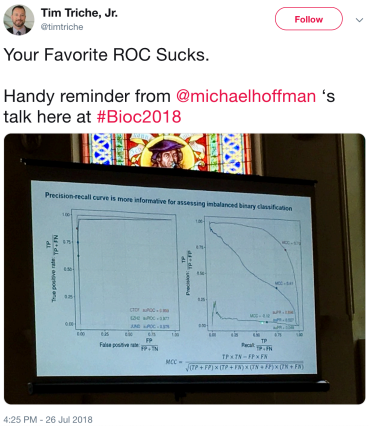
To interpret the AUC, you should know not just shat classifier was used, but how it was made into a collection of classifiers. You should also know whether it's a the area under an ROC curve, or a precision/recall curve.

ROC curve vs Precision-recall curve



source: https://twitter.com/timtriche/status/1022472947963969536

An alternative to the ROC is the precision recall curve. It works in exactly the same way, but has precision and recall on the axes.

As you can see, in many settings the latter can be much more informative, especially when you're a tally plotting the curves.. Practically, it's little effort to just plot both, and judge which one is more informative

setting the threshold

Show the user the ROC/PR curve, let them choose

This can be difficult to do accurately.

Estimate cost of misclassifications. Factor into the loss function. Minimize the expected cost.

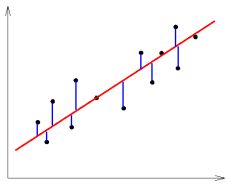
In sklearn, this is done by setting *class weights*. If a false negative costs as much as three false positives, we set the positive weight to 3 and the negative weight to 1.

The second approach works best with probabilistic classifiers, which we'll discuss next week.

break

"Up and left."

regression



loss function: (mean) squared errors

$$\frac{1}{n}\sum_i (\hat{y}_i - y_i)^2$$

evaluation function: root mean squared error

$$\sqrt{\frac{1}{n}\sum_i (\hat{y}_i - y_i)^2}$$

55

We'll quickly look at regression. We have much less to say here.

One thing to pay attention to is that if you use MSE loss, you may want to *report* the square root (the RMSE). The RMSE is minimised at the same places as the MSE, but it's easier to interpret, because it has the same units as the original output value.

For instance, if your outputs are in meters, then your MSE is measured in square meters, but your RMSE is also measured in meters.

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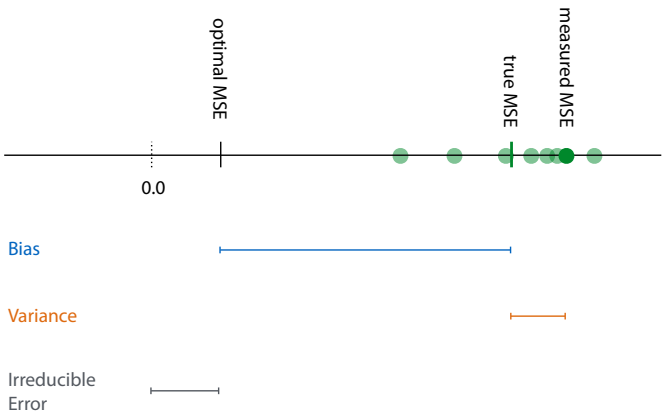
bias and variance



56

Normally, we train a regression model once, and get once MSE value. The lower the better. However this MSE is an estimate of the "true MSE" This is a value we can't compute, its the true expected performance of our entire method: from sampling data to training the model to computing the performance. If

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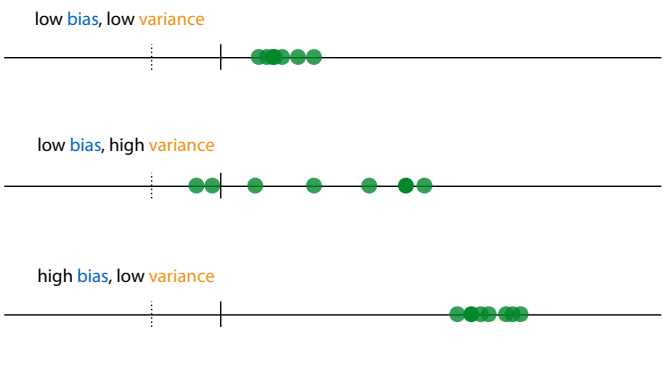
bias and variance



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bias and variance

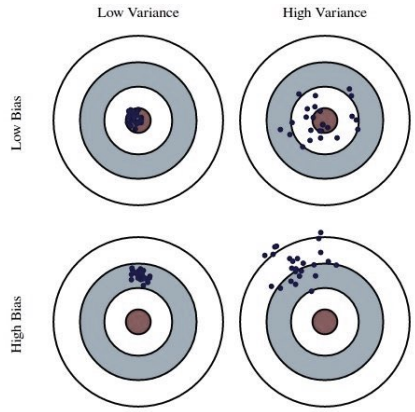

image source: http://scott.fortmann-roe.com/docs/BiasVariance.html (recommended reading)

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Remember, this is a metaphor for our RMSE error estimate. That means that normally, we have only one dart and we can't tell whether our error is due to high bias or high variance. We'll return to this topic in week 5, in the context of ensemble methods.

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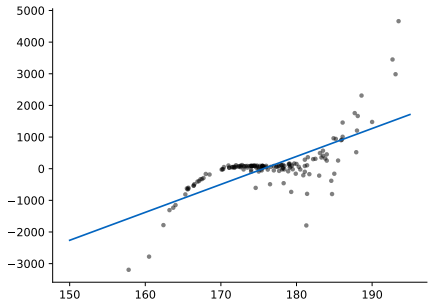
the bias-variance tradeoff

High bias: model doesn't fit the generating distribution. Poor assumptions, poor capacity.



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High bias tends to happen when the model can form the true shape of the data. Linear models in low-dimensional spaces often have this problem.

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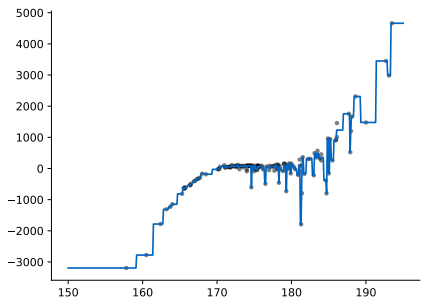
the bias-variance tradeoff

High variance: Sensitivity to random fluctuations, tendency to overfit.



60

High variance happens when the model has the capacity to follow the shape of the data perfectly, but so perfectly that it tends to get thrown off by small fluctuations.

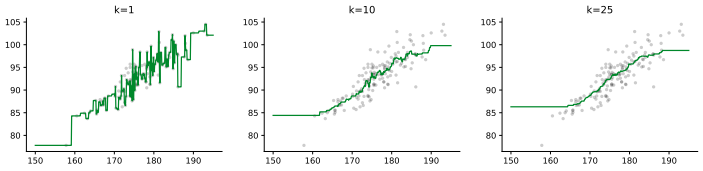
Even though this model (a regression tree) fits the data perfectly, if we resample the data, we are stuck with all sorts of weird peaks that won't fit the new data.

making the tradeoff

Reducing bias: increase model capacity, increase features.

Reducing variance: reduce model capacity, add regularization, reduce tree depth.

k-NN regression: increase k to increase bias, decrease variance.



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We will see techniques for all of these in the coming weeks. Note that often, it really is a tradeoff: reducing the bias, increases the variance and vice versa.

For some algorithms, there is a single parameter that allows us to make the bias/variance tradeoff. kNN is one example.

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week 5: ensembling

Combining models for variance reduction and for bias reduction.

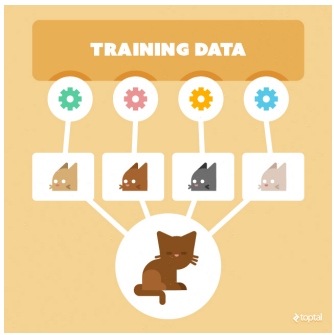

image source: https://www.toptal.com/machine-learning/ensemble-methods-machine-learning

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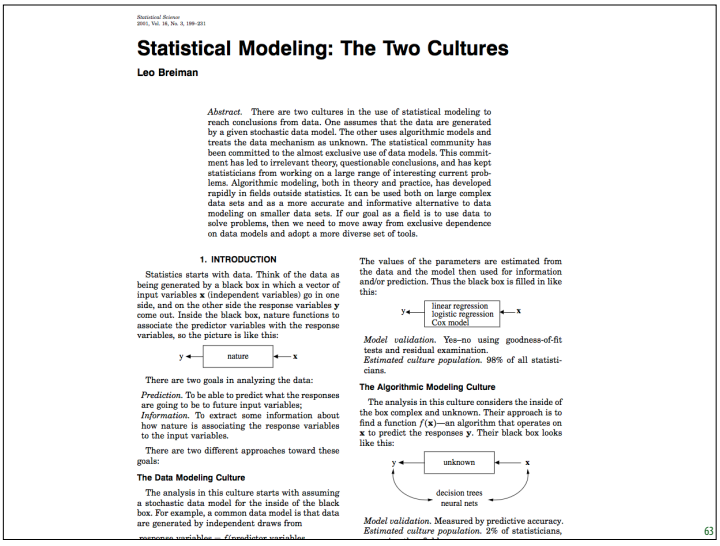
In week



Statistical Science
2001, Vol. 16, No. 3, 199–231

Statistical Modeling: The Two Cultures

Leo Breiman

Abstract. There are two cultures in the use of statistical modeling to reach conclusions from data. One assumes that the data are generated by a given stochastic data model. The other uses algorithmic models and treats the data mechanism as unknown. The statistical community has been committed to the almost exclusive use of data models. This commitment has led to irrelevant theory, questionable conclusions, and has kept statisticians from working on a large range of interesting current problems. Algorithmic modeling, both in theory and practice, has developed rapidly in fields outside statistics. It can be used both on large complex data sets and as a more accurate and informative alternative to data modeling on smaller data sets. If our goal as a field is to use data to solve problems, then we need to move away from exclusive dependence on data models and adopt a more diverse set of tools.

1. INTRODUCTION

Statistics starts with data. Think of the data as being generated by a black box in which a vector of input variables **x** (independent variables) go in one side, and on the other side the response variables **y** come out. Inside the black box, nature functions to associate the predictor variables with the response variables, so the picture is like this:

y ← nature ← x

There are two goals in analyzing the data:

Prediction. To be able to predict what the responses are going to be to future input variables;
Information. To extract some information about how nature is associating the response variables to the input variables.

There are two different approaches toward these goals:

The Data Modeling Culture

The analysis in this culture starts with assuming a stochastic data model for the inside of the black box. For example, a common data model is that data are generated by independent draws from

The values of the parameters are estimated from the data and the model then used for information and/or prediction. Thus the black box is filled in like this:

y ← linear regression / logistic regression / Cox model ← x

Model validation. Yes–no using goodness-of-fit tests and residual examination.
Estimated culture population. 98% of all statisticians.

The Algorithmic Modeling Culture

The analysis in this culture considers the inside of the box complex and unknown. Their approach is to find a function $f(\mathbf{x})$—an algorithm that operates on **x** to predict the responses **y**. Their black box looks like this:

y ← unknown ← x
decision trees / neural nets

Model validation. Measured by predictive accuracy.
Estimated culture population. 2% of statisticians,

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Given how much history and how many techniques we share with statistics, it's a little surprising how little statistical testing is done in ML research, and how reluctantly it is done when it is.

This paper by Leo Breiman shows the difference between the two cultures. It makes clear that the machine learning approach measuring models purely for predictive accuracy on a large test set, has a lot of benefits and makes the business of statistics a lot simple and more effective.

statistics for reported results

Can the observed results be attributed to *real characteristics* of the models under scrutiny or are they observed *by chance*?

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When it comes to reporting results, the question arises whether we should report our results with some sort of statistics. If we report that classifier A is better than classifier B because their accuracies are .997 and .998 respectively, can we really trust that statement? We've how much difference a little bit of noise can make, shouldn't we be reporting some kind of hypothesis test on that statement, to show that we've used enough test data?

quote source: ***http://www.icmla-conference.org/icmla11/PE_Tutorial.pdf***

should we do statistical tests at all?

- Makes ML experimentation difficult. Lots of disagreement.
- People overestimate the value of statistical analyses.
- Does not promote the best methods
- The ultimate validation of research is REPLICATION

On the appropriateness of statistical tests in machine learning, Janez Demšar,2008
Machine Learning as an Experimental Science (Revisited),Chris Drummond, 2006

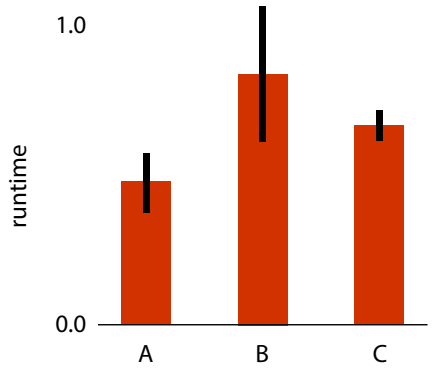
65

Note everybody agrees. Hypothesis testing comes with a lot of downsides. Given that we usually have very big sample sizes (10000 instances in the test set), our efforts may be better spent elsewhere.

Another consideration is that the ultimate validation of research is replication, not statistical significance. Somebody else should repeat your research and get the same results. Because all of our experimentation is computer code, a basic replication could be as simple as downloading and running a docker image. After that it's easy to try the same on new data, or check the model for bugs.

Since the community is so divided on the question, we won;won't emphasise reporting statistics on experimental results too much for this course. However, there are a few points worth mentioning.

error bars



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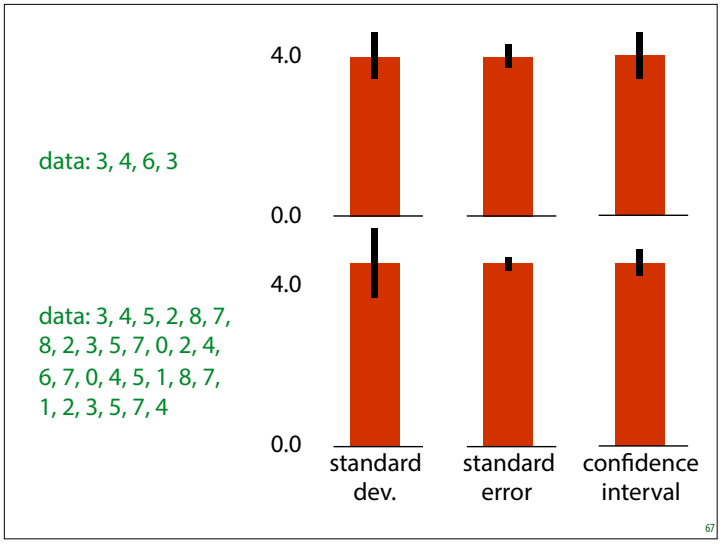
First, error bars.

If you see a picture like this, showing the mean runtime of an experiment, measured for three models, and averaged over a number of runs, what would you imagine the error bars denote?



The truth is, that there is no standard definition for what error bars denote, and if the authors didn't specify what their error bars indicate, the authors messed up.

These are the three most common options. Before we explain exactly what they mean, let's look at how they behave, specifically when we increase the amount of data.

If we sample more data, the estimate of our **standard deviation** becomes *more accurate*. It's an estimate of a property of our data distribution.

The standard error and the confidence interval are indicators of how confident we are about our estimate of the mean (indicated by the height of the error bar). There more data we have, *the smaller they get*.

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standard deviation:

- measure of **spread**, variance

standard error, confidence interval:

- measures of **confidence**

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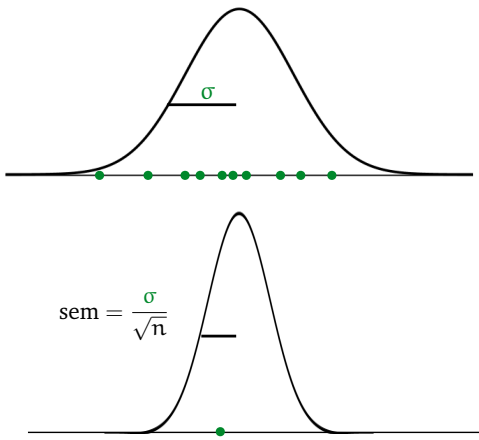
standard error

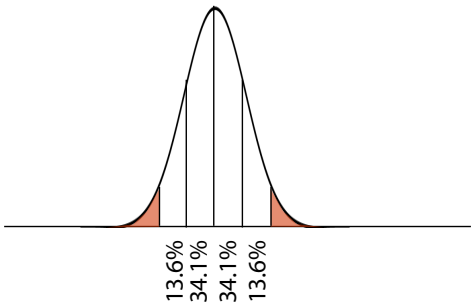


Here is how the standard error (SEM) works. If we sample some data (like error values) and calculate their mean, the result is random value too. If we resample, we get a (slightly) different mean. This means we can plot the probability distribution of this value.

If our original distribution is normal with standard deviation sigma, the distribution of the sample mean is approximately normal too (for large enough samples), with standard deviation sigma divided by the square of the number of samples.

The original standard deviation is not usually known, so it is estimated from the data. The bottom distribution is a Student's-t distribution. For large enough sample sizes (more than 100), we can treat this as a normal distribution.

95% confidence interval



mean +/- 1.96 sem is a 95% confidence interval

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As you may know, the region of four standard deviations around the mean of a normal distribution contains roughly 95% of the probability mass. This is what the confidence interval error bar is: it is simply twice the standard error on both sides of our estimate, and it gives us a region for which we are 95% confident that it contains the true mean.

---

about confidence intervals

Don't say: the probability that the true mean is in the confidence interval is 95%.

Do say: If we repeat the experiment many times, computing the confidence interval each time; the true mean would be inside the interval in 95% of those experiments.

The confidence interval changes from experiment to experiment, not the true mean.

The confidence interval for the mean is a statistic on the data, just like the mean itself or the standard deviation.

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This is an important distinction. These are frequentist methods, so there is no probability associated with the true mean at all. It is simply an objective, determined value (which we don't know). The probability comes from sampling, and from computing the interval from a sample.

So instead of having a fixed interval, with the true mean jumping around probabilistically, we have a fixed true mean around which we get an interval that jumps around if we resample the data The probability of it jumping so much that it no longer contains the true mean is 5%.

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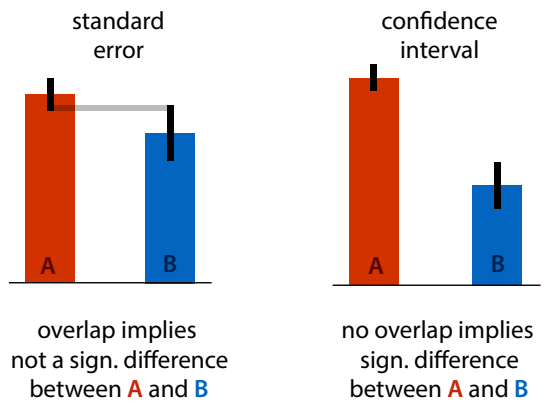
overlap



overlap implies not a sign. difference between A and B

no overlap implies sign. difference between A and B

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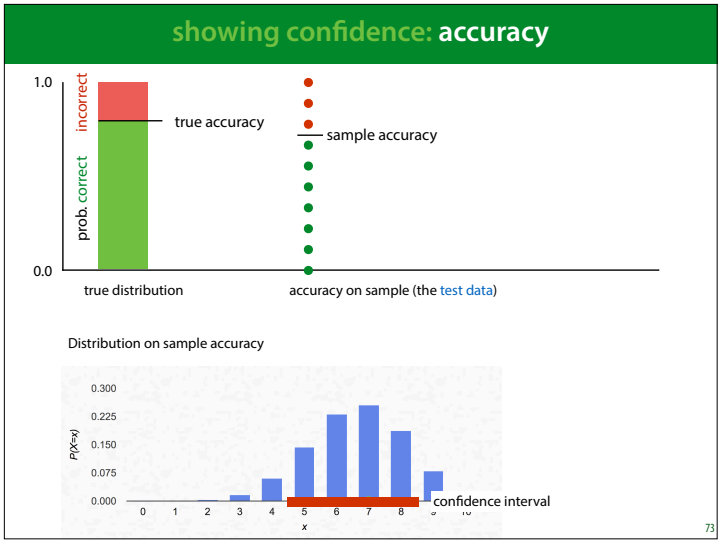
Say you plot the mean squared error for regression models **A** and **B**, together with some error bars. Does the the fact that the error bars overlap or not tell you whether the measured difference between the two models is statistically significant?

Yes, for standard error bars, the existence of overlap implies that there is no significant difference between the two effects (i.e. the possibility that the difference is due to random chance is high, and a repeat of the experiment on new data may show a different result). If you plot confidence interval error bars, and there is no overlap, you may conclude that the difference between the models is significant. If you repret the experiment on fresh data, it is very likely that model **A** would beat model **B** again.

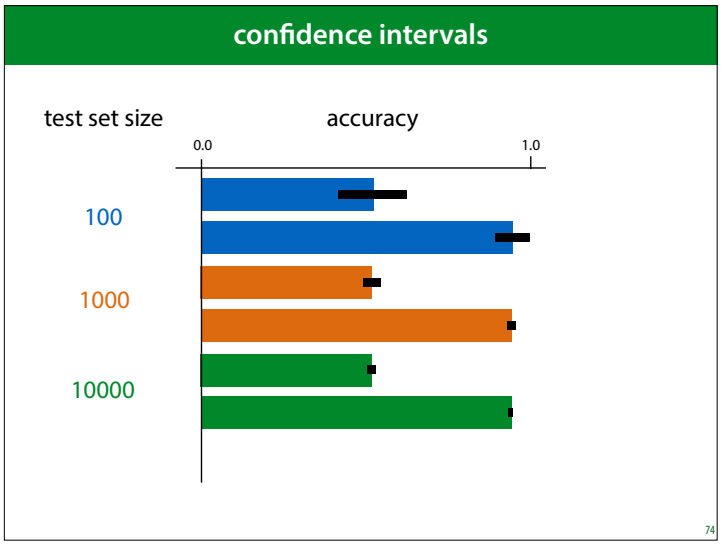
In both cases, the converse does not hold. If the SEM error bars do not overlap, there may or may not be a significant difference. If the confidence interval error bars do overlap, there may still be a significant difference, depending on how much they overlap.



The true accuracy of a classifier (the probability of a correct classification) is also one of these "true values", which we can't see, but that we estimate by a sample mean, where the sample is our test set. The accuracy that we actually see is an estimate of a true value. Each instance in our test set is like a flip of an unfair coin that lands heads for a correct classification and tails for an incorrect one. This is called a *Bernoulli* distribution.

Since this is a random process (our test set is randomly sampled), we can work out the distribution over the outcome (the number of correct classifications). The number of positive outcomes over a fixed-size sample from a Bernoulli distribution is described by a Binomial distribution. A region around our sample of 7 successes that contains 95% of the probability mass is a 95% confidence interval for our estimate of the accuracy.

This is the same process as shown on slide 67, but with a Bernoulli distribution instead of a Normal one.
source: ***https://homepage.divms.uiowa.edu/~mbognar/applets/bin.html***

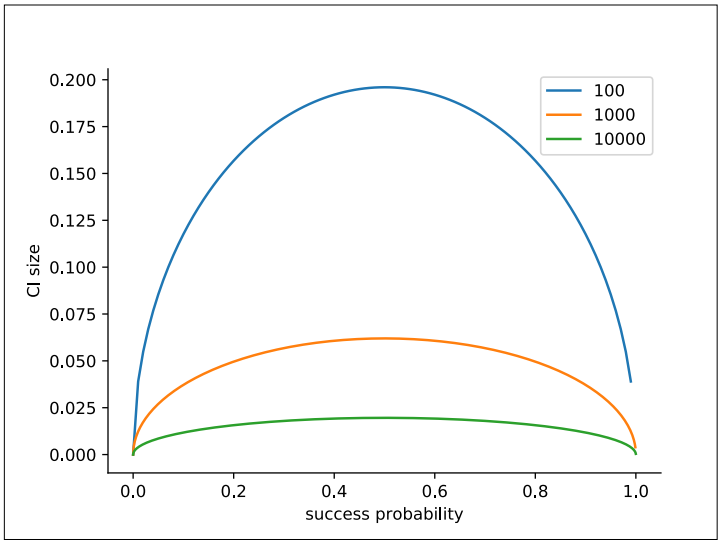


The size of this confidence interval depends on two factors: the true accuracy* and the size of the test set. Here are some examples for different accuracies and test set sizes.

This tells us that if the true success probability (accuracy) of a classifier is 0.5, and the test set contains 100 examples, our confidence interval has size 0.2. This means that even if we report 0.5 as the accuracy, we may well be wrong by as much as 0.1 either side.

Even if these confidence intervals are usually not reported, you can easily work them out (or look them up) yourself. So, if you see someone say that classifier A is better than classifier B because A scored 60% accuracy and and B score 59%, on a test set of 100 instances, you have reason to be sceptical.

We don't know the true accuracy, but it's accepted practice to assume that the estimate is close enough to get a reasonable estimate of the confidence interval.



Here are the full curves, in case you every need to look it up.

why use statistics in ML

- to show *confidence*
- to show *spread*

Confidently show the performance of the best model you found, and then measure the variance of the method you used to find it.

Showing confidence means showing how reliable our numbers are. Standard error and confidence intervals are good ways to show confidence (or lack thereof).

Showing spread is more about providing insight to the user. Say I train a classifier by gradient descent. If I have a big test set, I can very *confidently* measure and report the accuracy of this particular classifier. However, gradient descent uses *random* initialization. If I repeat the training process, I may end up in a different local minimum, and get a different classification performance. It's likely that I also want to communicate how much the measured performance is dependent on this randomness.

showing spread

Sources of randomness:

- Data sampling
- Search algorithm (i.e. initializing gradient descent)

Report standard deviation, describe *what* you repeat.

- How do you repeat data sampling?

If we have a large enough test set, we know that the confidence interval is small enough. But we do want to know how much the randomness in our process affects the result. What is the probability that repeating the process (on the same data, or on new data) produces wildly different results?

For factors like the initialisation of gradient descent, this is easy to test: you just rerun a few times on the same data. But how do you test how robust the result are against sampling a new dataset?

Resampling

Cross validation again, on the whole data set.

Stratified cross-validation (keeps the class proportions the same in all folds)

Leave-one-out cross-validation, a.k.a. the jackknife method

Slight bias: smaller datasets.

bootstrapping

Sample, with replacement, a dataset of the same size as the whole dataset.

On average, about 63.2% of the dataset will be included. The rest will be duplicated instances.

Each bootstrapped sample lets you repeat your experiment.

Note that some classifiers will respond poorly to presence of duplicate instances.

Better than cross validation for small datasets.

statistics: summary

Don't worry too much about it (until you have to).

Even in top ML conferences, rigorous statistical analysis is relatively rare.

Distinguish between showing *confidence*, and showing *spread*.

Think about what you want to claim, and what analysis would make your claim as strong as possible.

there's no free lunch

The no-free-lunch theorem(s)

Wolpert & MacReady 1997

"… any two optimization algorithms are equivalent when their performance is averaged across all possible problems"

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Given some data **X** and basic methods **A** and **B**?

Meta-methods:

- **method C**: Use cross validation, choose whichever performs the best.
- **method D**: Use cross validation, choose whichever performs the **worst**.

According to the NFL theorem, there are as many datasets X for which **C** beats **D** as there are for which **D** beats **C**.

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Note that, intuitively, method D would be an absolutely insane method to choose a model.

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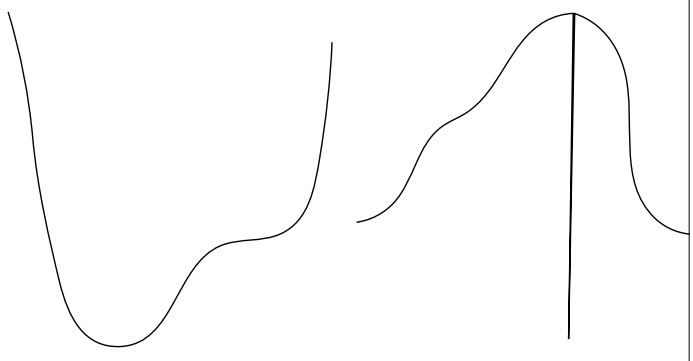
gradient descent



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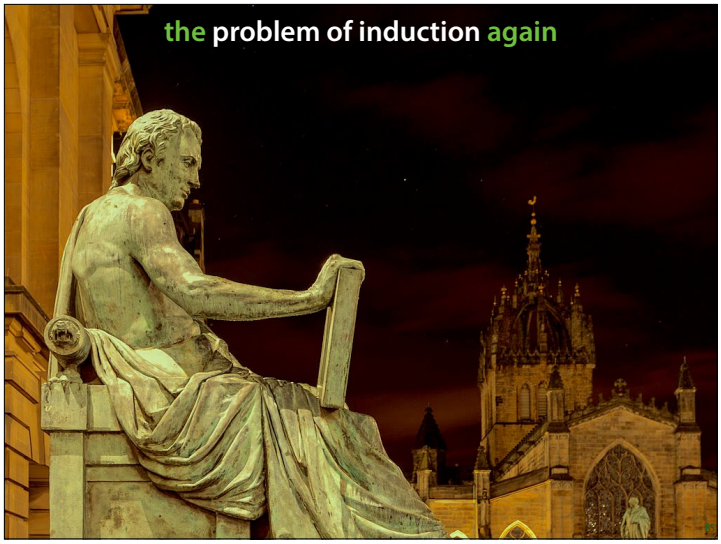
Here is another example. We know that gradient descent works well: to find the lowest point on a loss surface, you just follow the curve of the loss surface downward. However, for every loss surface and which gradient descent works, we can create a loss surface (like the one on the right) for which gradient ascent fails miserably, and actually, the opposite strategy works better: you have to climb to find the lowest point.



So we're back to the problem of induction. We can't prove that learning should work at all. And yet it seems to.

We need some assumption about the nature of the universe to understand why learning works at all.

The universal distribution

Not all datasets are created equal. The datasets for which our method works, are the likely ones.

The universe "generates" data for which our methods work

- Compressible data
- Simple data

The datasets that don't work aren't selected, because they look random to us.

We only understand those parts of the universe that generate understandable data

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One "out" to the NFL Theorem, is that there is a "universal distribution" governing the data gathering process. The NFL Theorem implicitly assumes that all datasets are equally likely. Since this is not the case, we can work out a universally best algorithm (under the universal distribution).

Occam's razor

"The simplest explanation is often the best"

We should bias our algorithms towards simple models.

- Reduces overfitting, helps generalization
- Why should this be the case? (Domingos, 1999)

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The no-free-lunch *principle*

There is no single best learning method. Whether an algorithm is good, depends on the domain.

Whether or not the NFL theorem means anything for us in practice, it has also given rise to a general *principle*, commonly followed in machine learning practice. The principle is that we should choose our method to deal with the task at hand, and not look for a universally best method.

Note that this is distinct from the NFT, because everybody still uses cross validation universally to evaluate *which of these many methods* is the best. And by the NFT cross-validation is also not a universal algorithm.

Inductive bias

The aspects of a learning algorithm, which implicitly or explicitly make it suitable for certain learning problems and unsuitable for others.

A linear method has an *inductive bias* for linear relations.

warning: group sessions coming up

Next thursday for half of the groups (check Canvas).


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